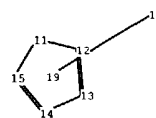
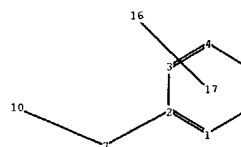
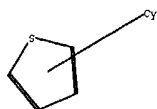
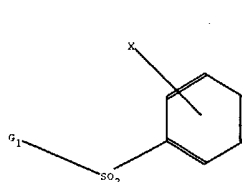


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chain nodes :

7 10 16 18

ring nodes :

1 2 3 4 5 6 11 12 13 14 15

chain bonds :

2-7 7-10

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

7-10

exact bonds :

2-7 11-12 11-15 12-13 13-14 14-15

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

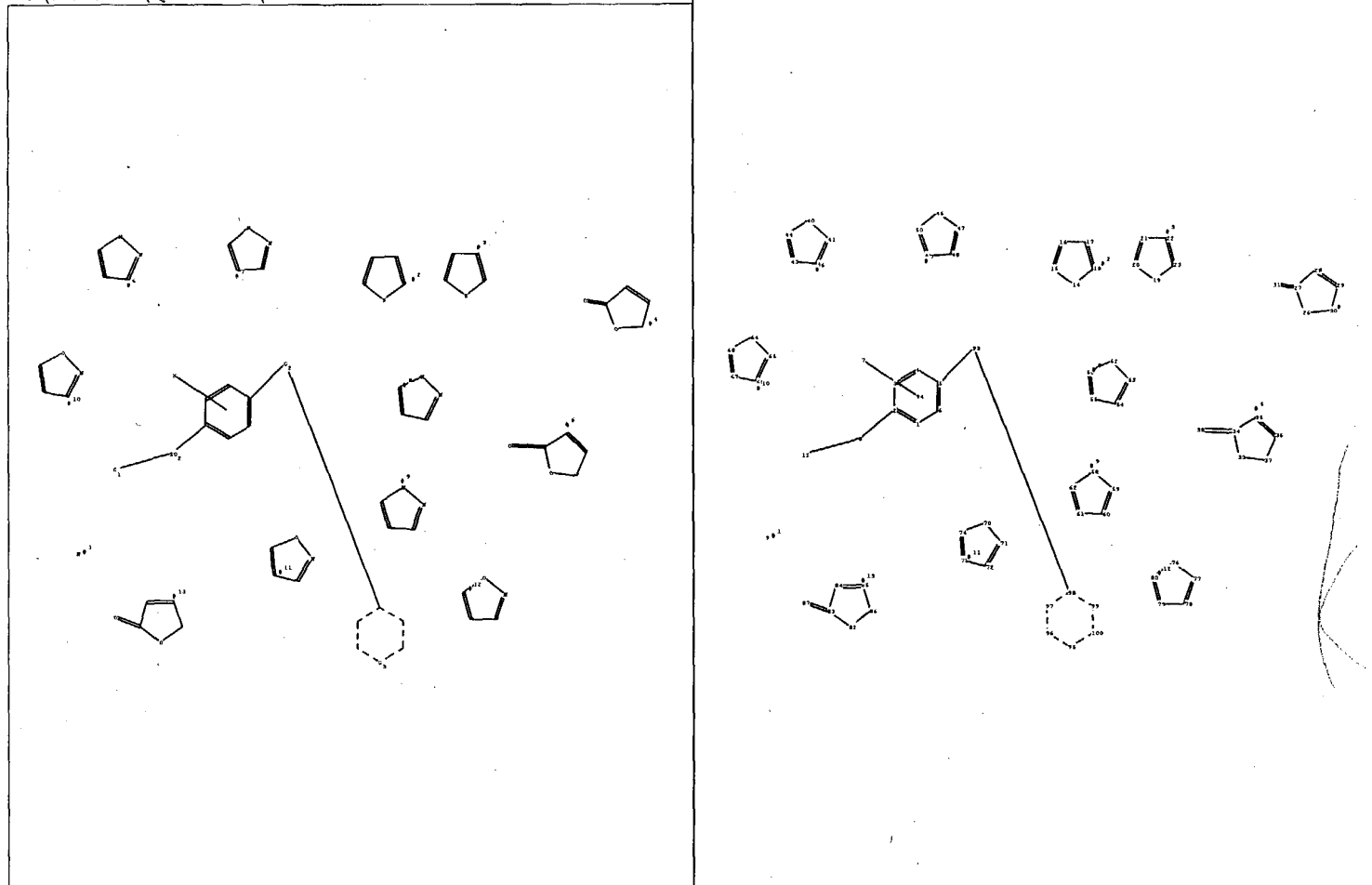
isolated ring systems :

containing 1 : 11 :

G1:Ak,NH2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 10:CLASS 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:Atom 19:CLASS



chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
 36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
 64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 95 96
 97 98 99 100

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-98

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
 21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
 40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
 55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
 71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 84-85 85-86
 95-96 95-100 96-97 97-98 98-99 99-100

exact/norm bonds :

5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54
 58-59 58-62 59-60 65-66 71-72 77-78 83-87 93-98 95-96 95-100 96-97 97-98
 98-99 99-100

exact bonds :

2-8 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30
 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 42-43 43-44 48-49 49-50 54-55
 55-56 60-61 61-62 64-65 64-68 66-67 67-68 70-71 70-74 72-73 73-74 76-77 76-80
 78-79 79-80 82-83 82-86 83-84 84-85 85-86

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

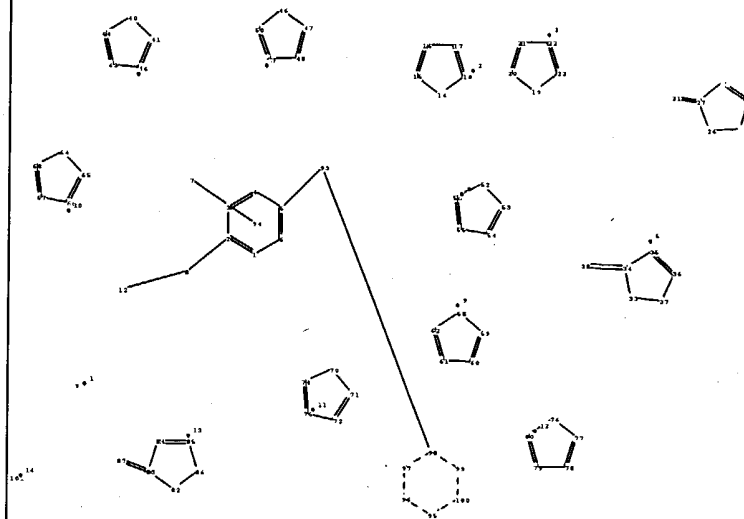
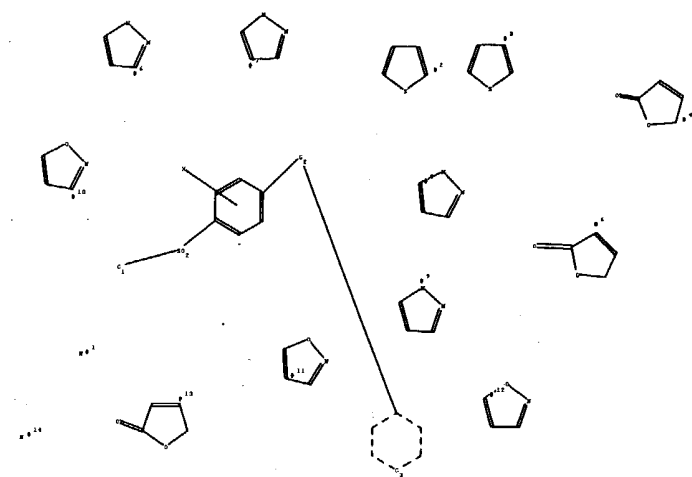
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 100:Atom



chain nodes :

7 8 9 12 31 38 87 93 101

ring nodes :

1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 95 96
97 98 99 100

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-98

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 84-85 85-86
95-96 95-100 96-97 97-98 98-99 99-100

exact/norm bonds :

5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54
58-59 58-62 59-60 65-66 71-72 77-78 83-87 93-98 95-96 95-100 96-97 97-98
98-99 99-100

exact bonds :

2-8 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30
27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 42-43 43-44 48-49 49-50 54-55
55-56 60-61 61-62 64-65 64-68 66-67 67-68 70-71 70-74 72-73 73-74 76-77 76-80
78-79 79-80 82-83 82-86 83-84 84-85 85-86

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

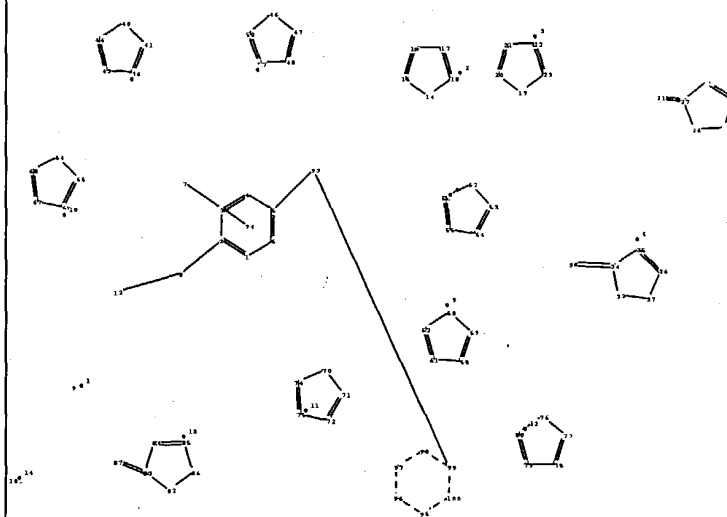
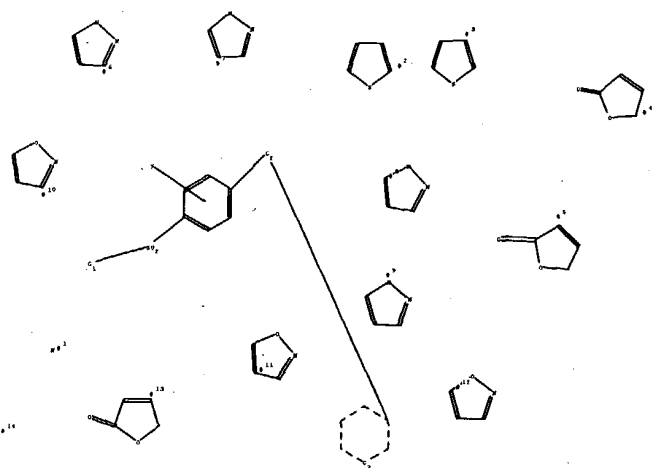
:CH3,Et,[*1]

: [*2], [*3], [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13]

G3:C,[*14]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 100:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93 101

ring nodes :

1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
 36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
 64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 95 96
 97 98 99 100

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-99

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
 21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
 40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
 55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
 71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 84-85 85-86
 95-96 95-100 96-97 97-98 98-99 99-100

exact/norm bonds :

5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54
 58-59 58-62 59-60 65-66 71-72 77-78 83-87 93-99 95-96 95-100 96-97 97-98
 98-99 99-100

exact bonds :

2-8 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30
 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 42-43 43-44 48-49 49-50 54-55
 55-56 60-61 61-62 64-65 64-68 66-67 67-68 70-71 70-74 72-73 73-74 76-77 76-80
 78-79 79-80 82-83 82-86 83-84 84-85 85-86

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

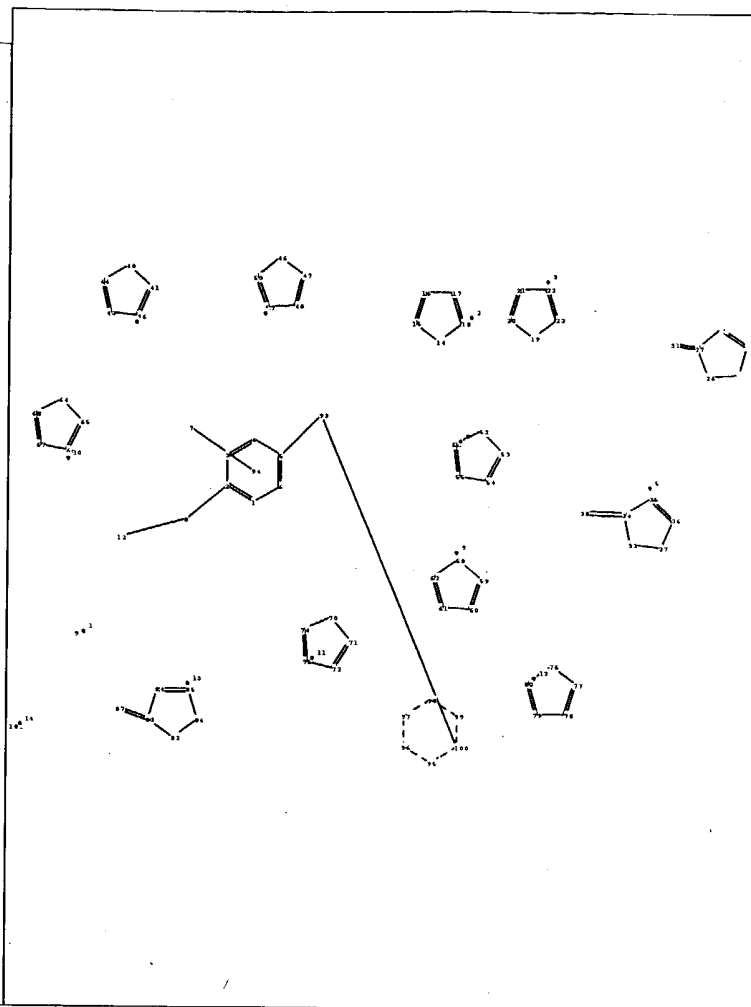
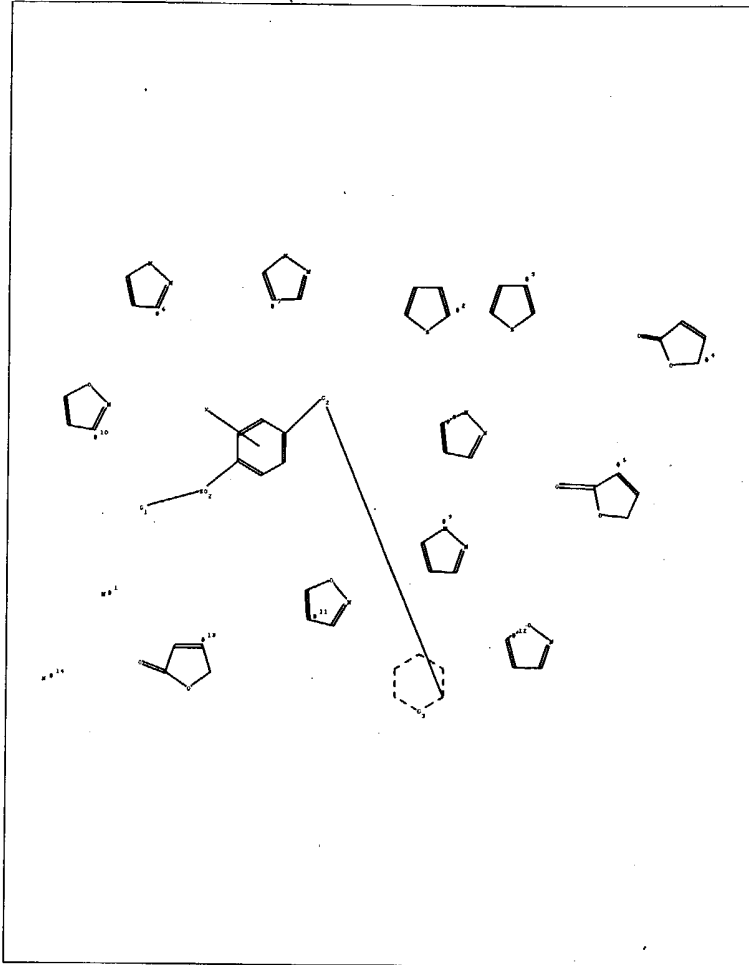
1:CH3,Et,[*1]

2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C, [*14]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
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85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 100:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93 101

ring nodes :

1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
 36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
 64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 95 96
 97 98 99 100

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-100

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
 21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
 40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
 55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
 71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 84-85 85-86
 95-96 95-100 96-97 97-98 98-99 99-100

exact/norm bonds :

5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54
 58-59 58-62 59-60 65-66 71-72 77-78 83-87 93-100 95-96 95-100 96-97 97-98
 98-99 99-100

exact bonds :

2-8 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30
 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 42-43 43-44 48-49 49-50 54-55
 55-56 60-61 61-62 64-65 64-68 66-67 67-68 70-71 70-74 72-73 73-74 76-77 76-80
 78-79 79-80 82-83 82-86 83-84 84-85 85-86

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

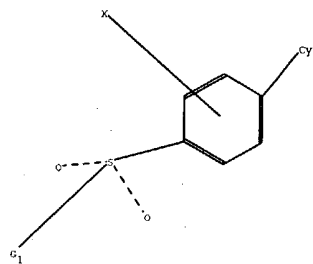
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

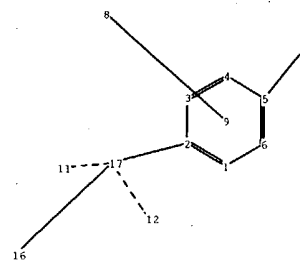
c, [*14]

ch level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 100:Atom 101:CLASS



10¹



10¹

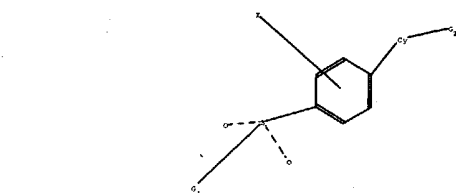
```

chain nodes :
  7  8 11 12 13 16 17
ring nodes :
  1  2  3  4  5  6
chain bonds :
  2-17  5-7 11-17 12-17 16-17
ring bonds :
  1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
  2-17  5-7 11-17 12-17 16-17
normalized bonds :
  1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
  containing 1 :
  
```

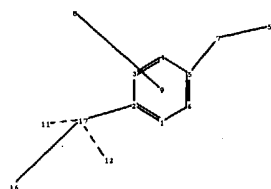
G1:CH3,Et,[*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS 16:CLASS 17:CLASS



H 1



H 1



chain nodes :

7 8 11 12 13 16 17 54

ring nodes :

1 2 3 4 5 6 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35
36 37 38 39 40 41 42 43 44 45 46 47

chain bonds :

2-17 5-7 7-54 11-17 12-17 16-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23 24-25 24-29
25-26 26-27 27-28 28-29 30-31 30-35 31-32 32-33 33-34 34-35 36-37 36-41 37-38
38-39 39-40 40-41 42-43 42-47 43-44 44-45 45-46 46-47

exact/norm bonds :

2-17 5-7 7-54 11-17 12-17 16-17

exact bonds :

18-19 18-23 19-20 20-21 21-22 22-23

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 24-25 24-29 25-26 26-27 27-28 28-29 30-31 30-35
31-32 32-33 33-34 34-35 36-37 36-41 37-38 38-39 39-40 40-41 42-43 42-47 43-44
44-45 45-46 46-47

isolated ring systems :

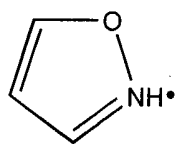
containing 1 : 18 : 24 : 30 : 36 : 42 :

G1:CH3,Et,[*1]

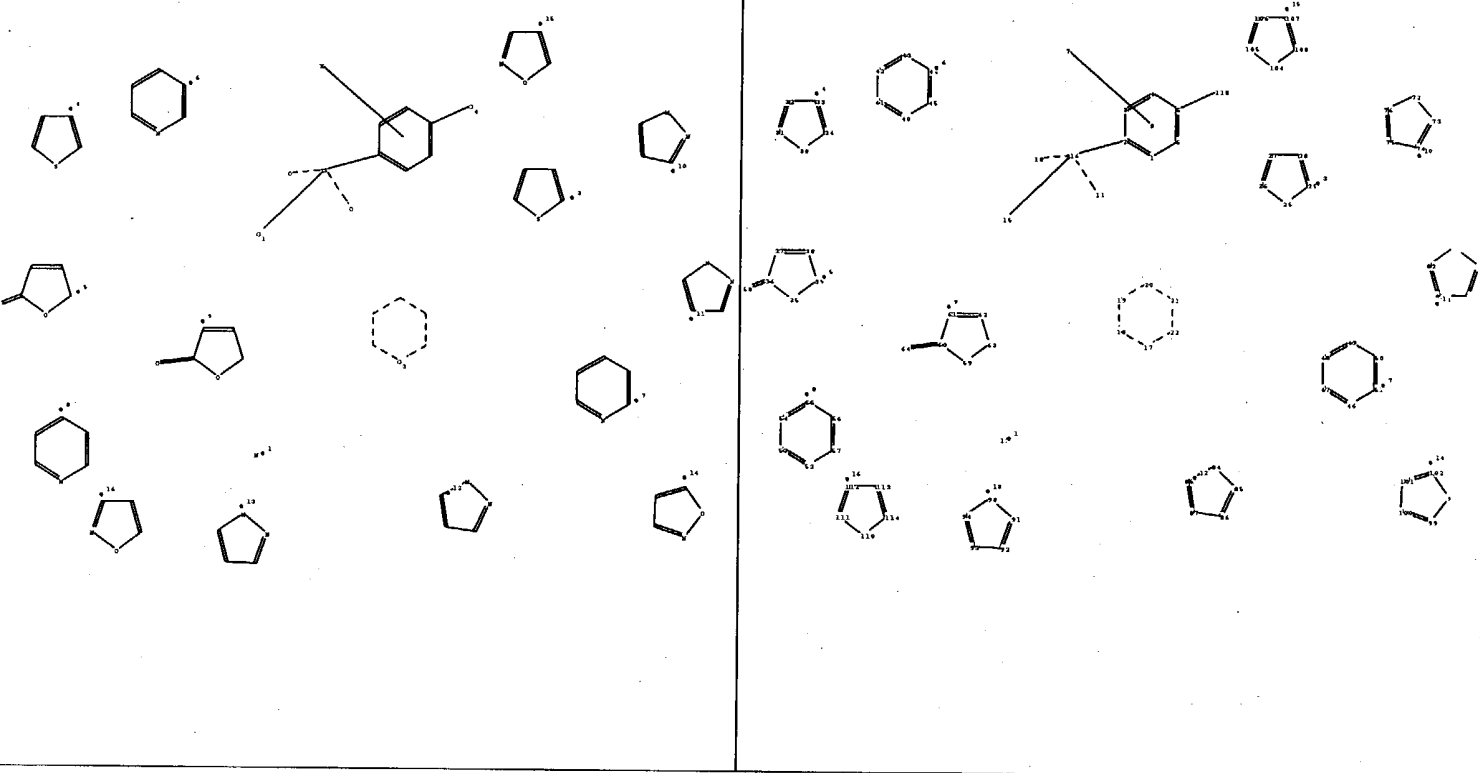
G2:[*2],[*3],[*4],[*5],[*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom
43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 54:CLASS



isoxazoly



chain nodes :

7 10 11 12 15 16 58 64 118

ring nodes :

1 2 3 4 5 6 17 18 19 20 21 22 25 26 27 28 29 30 31 32 33 34 35 36
 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 59
 60 61 62 63 72 73 74 75 76 78 79 80 81 82 84 85 86 87 88 90 91 92
 93 94 98 99 100 101 102 104 105 106 107 108 110 111 112 113 114

chain bonds :

2-16 5-118 10-16 11-16 15-16 36-58 60-64

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22 25-26 25-29
 26-27 27-28 28-29 30-31 30-34 31-32 32-33 33-34 35-36 35-39 36-37 37-38 38-39
 40-41 40-45 41-42 42-43 43-44 44-45 46-47 46-51 47-48 48-49 49-50 50-51 52-53
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 74-75 75-76 78-79 78-82 79-80 80-81 81-82 84-85 84-88 85-86 86-87 87-88 90-91
 90-94 91-92 92-93 93-94 98-99 98-102 99-100 100-101 101-102 104-105 104-108
 105-106 106-107 107-108 110-111 110-114 111-112 112-113 113-114

exact/norm bonds :

2-16 5-118 10-16 11-16 15-16 17-18 17-22 18-19 19-20 20-21 21-22 25-26 25-29
 26-27 27-28 28-29 30-31 30-34 31-32 32-33 33-34 35-36 35-39 36-37 36-58 37-38
 38-39 59-60 59-63 60-61 60-64 61-62 62-63 72-73 72-76 73-74 74-75 75-76 78-79
 78-82 79-80 80-81 81-82 84-85 84-88 85-86 86-87 87-88 90-91 90-94 91-92 92-93
 93-94 98-99 98-102 99-100 100-101 101-102 104-105 104-108 105-106 106-107
 107-108 110-111 110-114 111-112 112-113 113-114

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 40-41 40-45 41-42 42-43 43-44 44-45 46-47 46-51
 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56 56-57

isolated ring systems :

containing 1 : 17 : 25 : 30 : 35 : 40 : 46 : 52 : 59 : 72 : 78 : 84 : 90 : 110 :

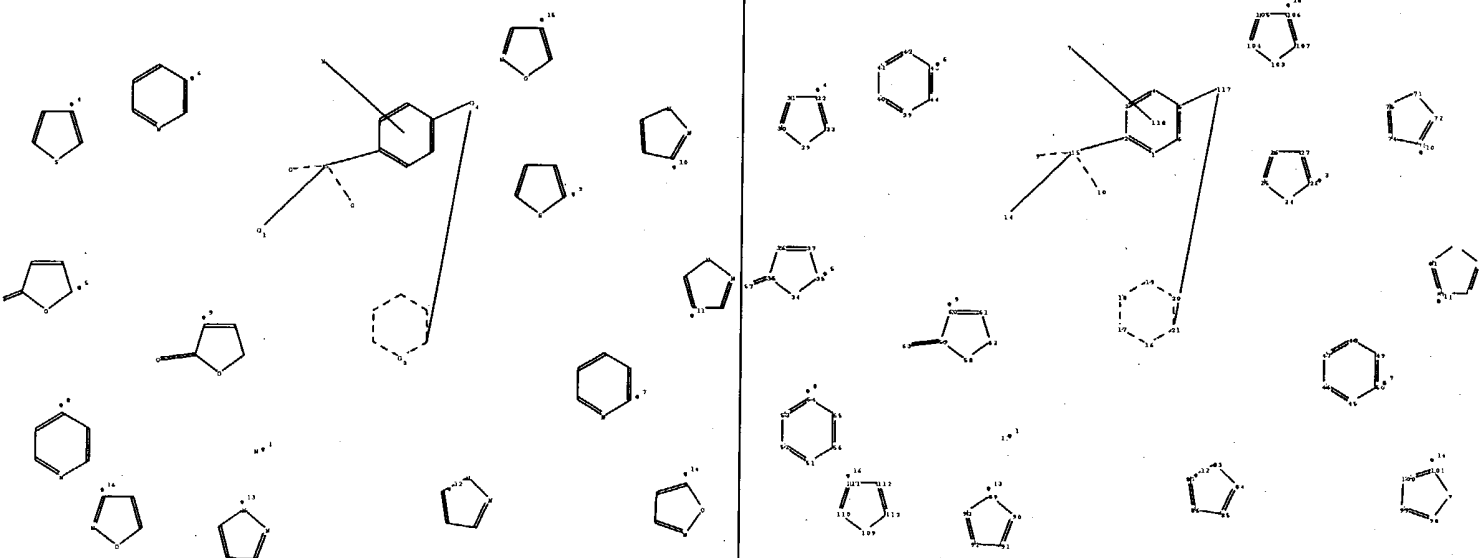
1:CH3,Et,[*1]

G3:C,N

G4:[*1],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15],[*16]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS
12:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom
45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:CLASS
54:CLASS 55:Atom 56:Atom 57:Atom 58:CLASS 59:Atom 60:Atom 61:Atom 62:Atom
63:Atom 64:CLASS 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 78:Atom 79:Atom 80:Atom
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93:Atom 94:Atom 98:Atom 99:Atom 100:Atom 101:Atom 102:Atom 104:Atom 105:Atom
106:Atom 107:Atom 108:Atom 110:Atom 111:Atom 112:Atom 113:Atom 114:Atom 118:CLASS



chain nodes :

7 9 10 11 14 15 57 63 117

ring nodes :

1 2 3 4 5 6 16 17 18 19 20 21 24 25 26 27 28 29 30 31 32 33 34 35
 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 58
 59 60 61 62 71 72 73 74 75 77 78 79 80 81 83 84 85 86 87 89 90 91
 92 93 97 98 99 100 101 103 104 105 106 107 109 110 111 112 113

chain bonds :

2-15 5-117 9-15 10-15 14-15 21-117 35-57 59-63

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 24-25 24-28
 25-26 26-27 27-28 29-30 29-33 30-31 31-32 32-33 34-35 34-38 35-36 36-37 37-38
 39-40 39-44 40-41 41-42 42-43 43-44 45-46 45-50 46-47 47-48 48-49 49-50 51-52
 51-56 52-53 53-54 54-55 55-56 58-59 58-62 59-60 60-61 61-62 71-72 71-75 72-73
 73-74 74-75 77-78 77-81 78-79 79-80 80-81 83-84 83-87 84-85 85-86 86-87 89-90
 89-93 90-91 91-92 92-93 97-98 97-101 98-99 99-100 100-101 103-104 103-107
 104-105 105-106 106-107 109-110 109-113 110-111 111-112 112-113

exact/norm bonds :

2-15 5-117 9-15 10-15 14-15 16-17 16-21 17-18 18-19 19-20 20-21 21-117 24-25
 24-28 25-26 26-27 27-28 29-30 29-33 30-31 31-32 32-33 34-35 34-38 35-36 35-57
 36-37 37-38 58-59 58-62 59-60 59-63 60-61 61-62 71-72 71-75 72-73 73-74 74-75
 77-78 77-81 78-79 79-80 80-81 83-84 83-87 84-85 85-86 86-87 89-90 89-93 90-91
 91-92 92-93 97-98 97-101 98-99 99-100 100-101 103-104 103-107 104-105 105-106
 106-107 109-110 109-113 110-111 111-112 112-113

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 39-40 39-44 40-41 41-42 42-43 43-44 45-46 45-50
 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56

isolated ring systems :

containing 1 : 16 : 24 : 29 : 34 : 39 : 45 : 51 : 58 : 71 : 77 : 83 : 89 : 109 :

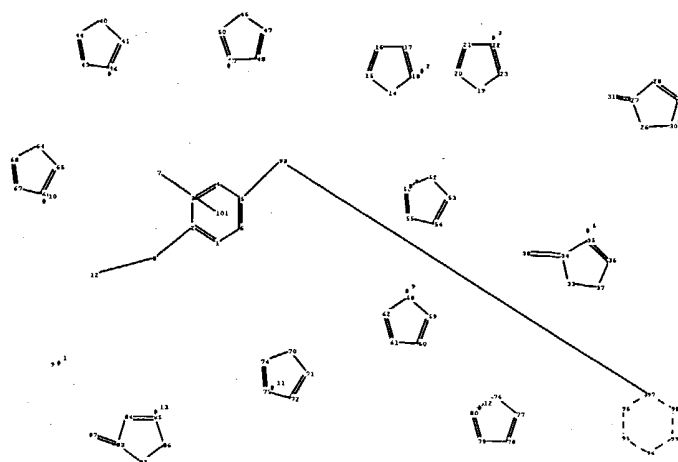
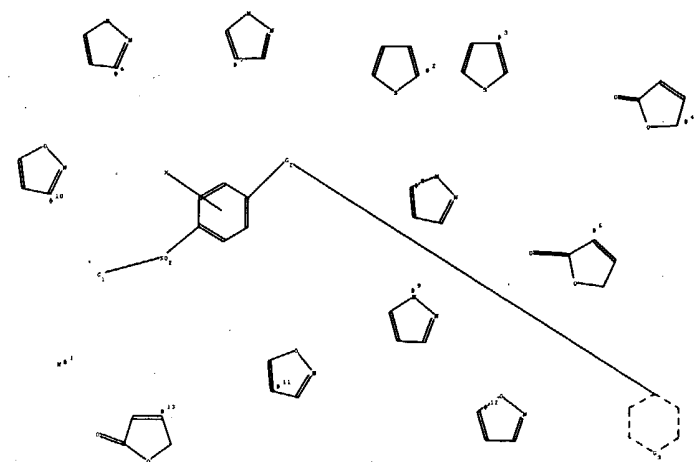
1:CH3,Et,[*1]

G3:C,N

G4:[*1],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15],[*16]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS
14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom
45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom
55:Atom 56:Atom 57:CLASS 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS
71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom
83:Atom 84:Atom 85:Atom 86:Atom 87:Atom 89:Atom 90:Atom 91:Atom 92:Atom 93:Atom
97:Atom 98:Atom 99:Atom 100:Atom 101:Atom 103:Atom 104:Atom 105:Atom 106:Atom
107:Atom 109:Atom 110:Atom 111:Atom 112:Atom 113:Atom 117:CLASS 118:CLASS



main nodes :

7 8 9 12 31 38 87 93

ing nodes :

1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 94 95
96 97 98 99

main bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-97

ing bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 84-85 85-86
94-95 94-99 95-96 96-97 97-98 98-99

act/norm bonds :

2-8 5-93 8-12 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23
26-27 26-30 27-28 27-31 28-29 29-30 33-34 33-37 34-35 34-38 35-36 36-37 40-41
40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 83-87 84-85
85-86 93-97 94-95 94-99 95-96 96-97 97-98 98-99

rmalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

olated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

:CH3,Et,[*1]

: [*2], [*3], [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13]

:C,N

Match level :

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 101:CLASS
```

C:\stnweb\Queries\5b.str

chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 94 95
96 97 98 99

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-98

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 84-85 85-86
94-95 94-99 95-96 96-97 97-98 98-99

exact/norm bonds :

2-8 5-93 8-12 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23
26-27 26-30 27-28 27-31 28-29 29-30 33-34 33-37 34-35 34-38 35-36 36-37 40-41
40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 83-87 84-85
85-86 93-98 94-95 94-99 95-96 96-97 97-98 98-99

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

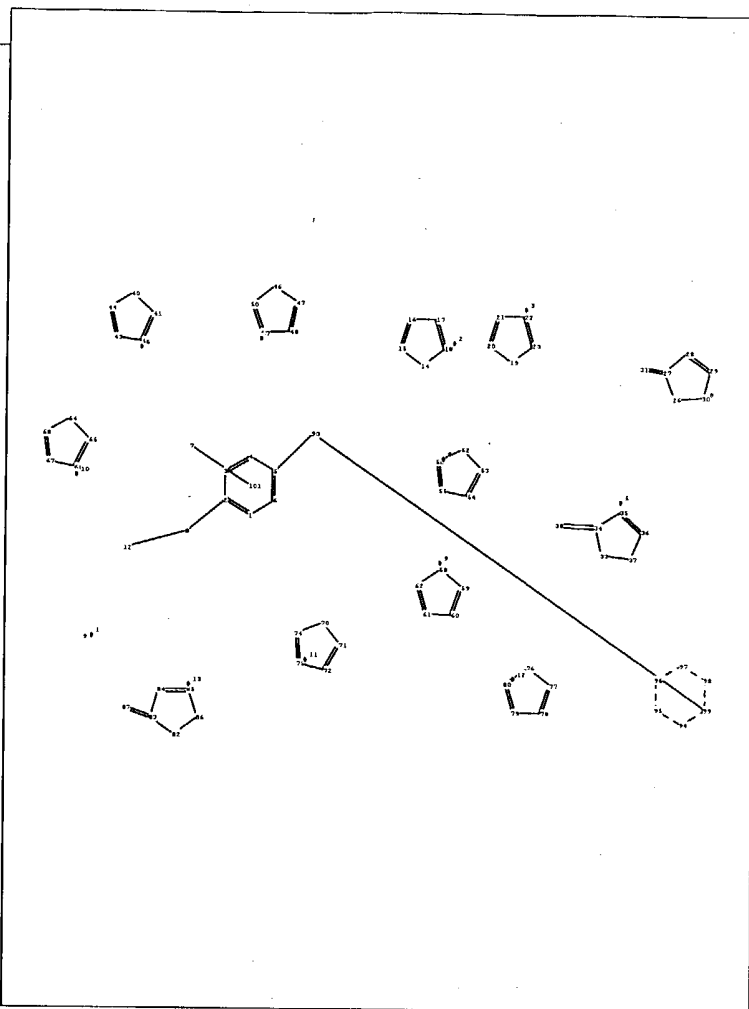
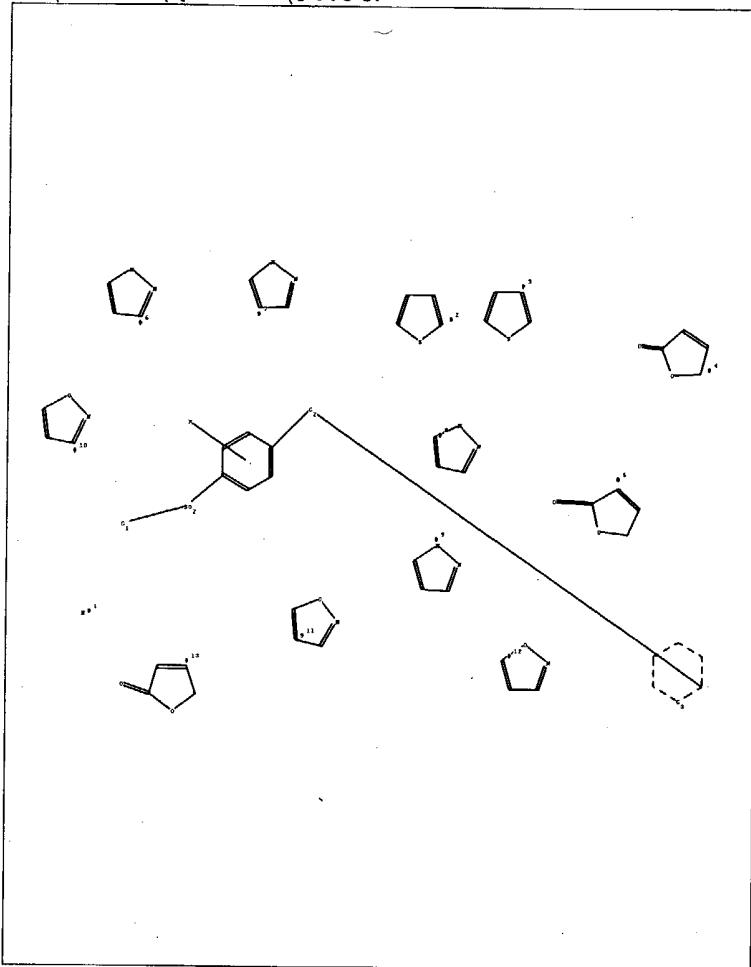
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
 36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
 64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 94 95
 96 97 98 99

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-99

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
 21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
 40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
 55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
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exact/norm bonds :

2-8 5-93 8-12 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23
 26-27 26-30 27-28 27-31 28-29 29-30 33-34 33-37 34-35 34-38 35-36 36-37 40-41
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 55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
 71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 83-87 84-85
 85-86 93-99 94-95 94-99 95-96 96-97 97-98 98-99

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

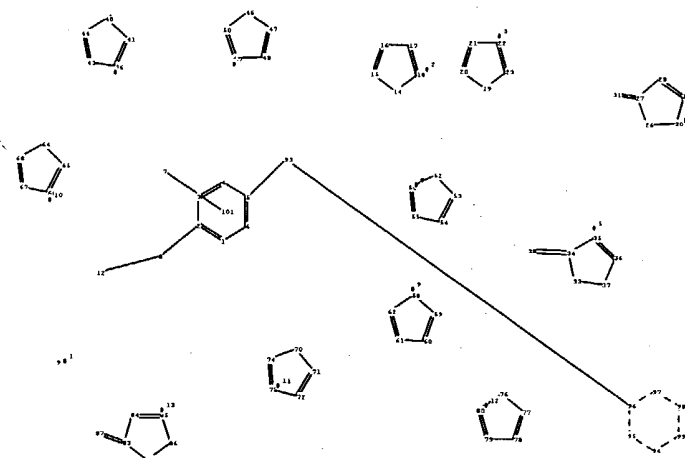
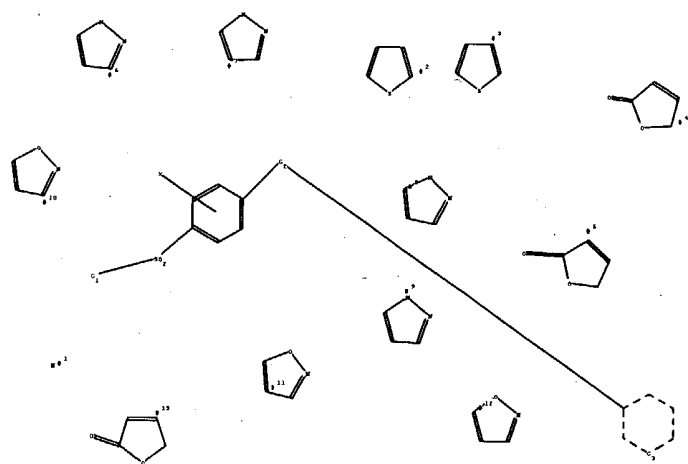
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

atch level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
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49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
 36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
 64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 94 95
 96 97 98 99

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-96

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
 21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
 40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
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exact/norm bonds :

2-8 5-93 8-12 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23
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 85-86 93-96 94-95 94-99 95-96 96-97 97-98 98-99

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

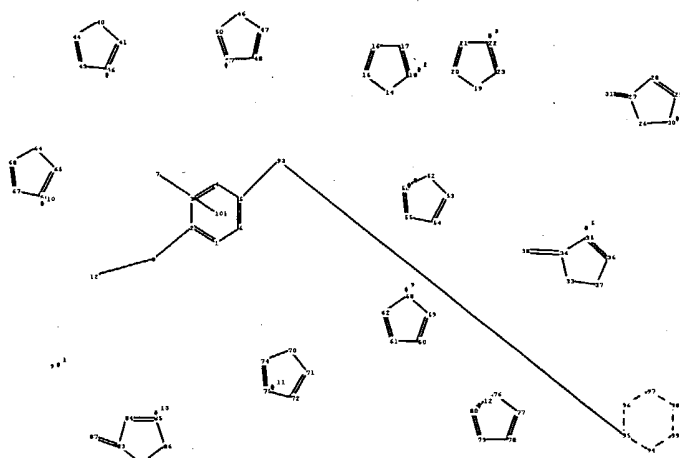
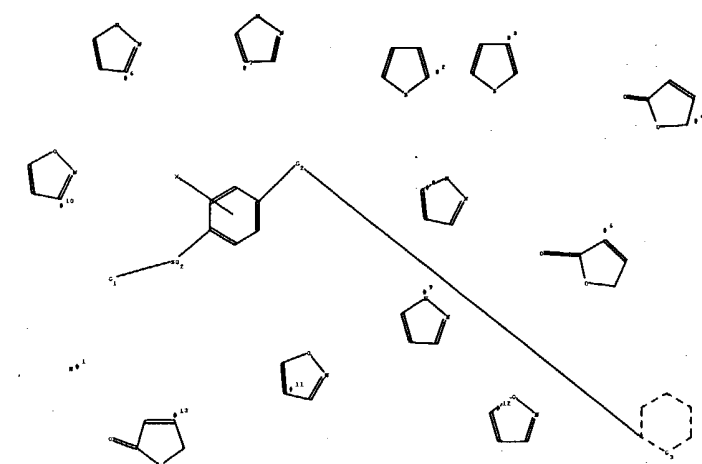
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
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73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
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chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
 36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
 64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 94 95
 96 97 98 99

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-95

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
 21-22 22-23 26-27 26-30 27-28 27-31 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
 40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
 55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
 71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 84-85 85-86
 94-95 94-99 95-96 96-97 97-98 98-99

exact/norm bonds :

2-8 5-93 8-12 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23
 26-27 26-30 27-28 27-31 28-29 29-30 33-34 33-37 34-35 34-38 35-36 36-37 40-41
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 71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 83-87 84-85
 85-86 93-95 94-95 94-99 95-96 96-97 97-98 98-99

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

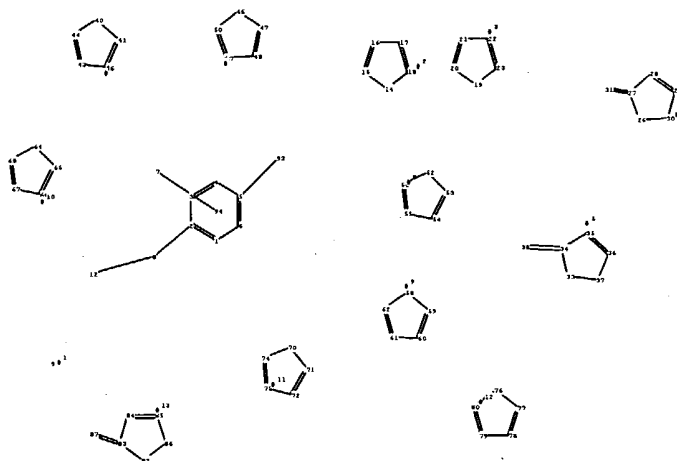
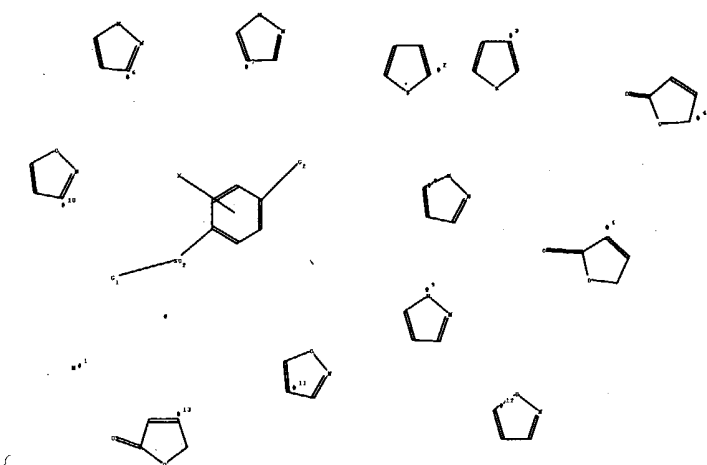
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
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85:Atom 86:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1 2 3 4 5 6 14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
 36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
 64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
 21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
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 71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 84-85 85-86

exact/norm bonds :

5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54
 58-59 58-62 59-60 65-66 71-72 77-78 83-87

exact bonds :

2-8 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30
 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 42-43 43-44 48-49 49-50 54-55
 55-56 60-61 61-62 64-65 64-68 66-67 67-68 70-71 70-74 72-73 73-74 76-77 76-80
 78-79 79-80 82-83 82-86 83-84 84-85 85-86

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
 14:Atom

	15:Atom	16:Atom	17:Atom	18:Atom	19:Atom	20:Atom	21:Atom	22:Atom	23:Atom
26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	31:CLASS	33:Atom	34:Atom	35:Atom	36:Atom
37:Atom	38:CLASS	40:Atom	41:Atom	42:Atom	43:Atom	44:Atom	46:Atom	47:Atom	48:Atom
49:Atom	50:Atom	52:Atom	53:Atom	54:Atom	55:Atom	56:Atom	58:Atom	59:Atom	60:Atom
61:Atom	62:Atom	64:Atom	65:Atom	66:Atom	67:Atom	68:Atom	70:Atom	71:Atom	72:Atom
73:Atom	74:Atom	76:Atom	77:Atom	78:Atom	79:Atom	80:Atom	82:Atom	83:Atom	84:Atom
85:Atom	86:Atom	87:CLASS	93:CLASS	94:CLASS					